Lithium Diffusion in Amorphous Lithium-Silicon

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In order to further the development of novel negative electrode materials for lithium-ion batteries, understanding the basic principles of atomic transport is of high importance. Amorphous silicon is a very interesting high-capacity negative electrode material for innovative applications. Amorphous lithium-silicon (Li_xSi) is formed during lithiation of silicon electrodes but can also be directly used as electrode material. In both cases the lithium diffusion properties influence the achievable (dis-)charging rates, the maximum capacity and the mechanical stress formation.

Thin Li_xSi films were investigated, which were produced by ion-beam co-sputtering of segmented elemental Li and Si targets. This allows a variation of the Li fraction in Li_xSi films between $0.05 < x < 0.5$ [1]. For the experiments $^{6}Li_xSi/^{nat}Li_xSi$ isotope heterostructures were deposited and interdiffusion of ^{6}Li and ^{7}Li isotopes was analysed by secondary ion mass spectrometry before and after annealing. Diffusivities were extracted by comparing the experimental isotope depth profiles to analytical solutions of the diffusion equation. The diffusivities of $Li_{0.1}Si$ follow the Arrhenius law between 140 and 300 °C with an activation energy of 1.4 eV and a pre-exponential factor of $2 \cdot 10^{-5}$ $m^2 \cdot s^{-1}$. This points to a trap-limited diffusion mechanism. In contrast, for $Li_{0.4}Si$ complete isotope interdiffusion is observed directly after deposition at room temperature. These results indicate an acceleration of diffusion with increasing Li content as suggested in literature [2].

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